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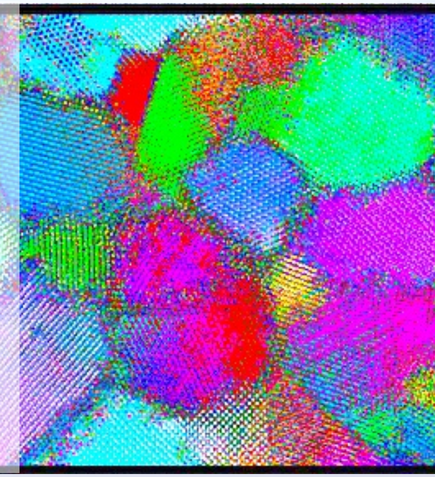


Sandia's modeling of tantalum strength

J. Matthew D. Lane

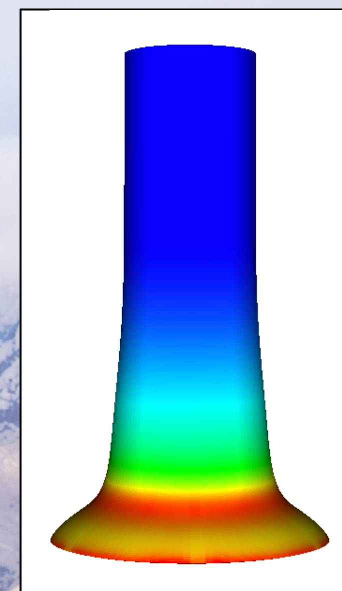
Sandia National Laboratories,

Albuquerque, NM

Atomistic: **Alex Moore**, Chris Weinberger, Fadi Abdeljawad, Stephen Foiles

Meso & continuum: **Hojun Lim**, **Corbett Battaile**

Experiments: Thomas Buchheit, Jay Carroll, Brad Boyce, **Justin L. Brown**



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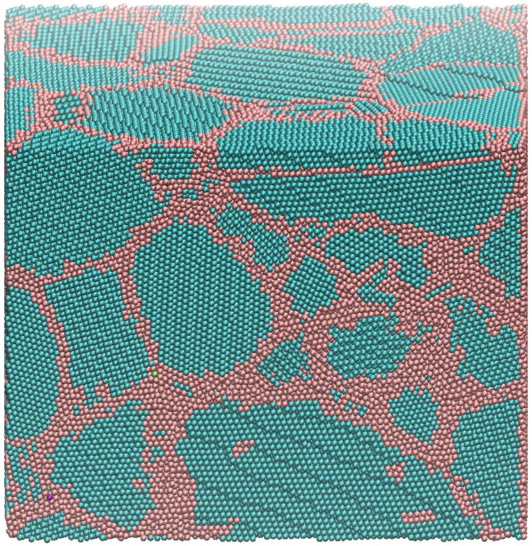
Sandia's modeling approach

Sandia is currently pursuing strength modeling at multiple length and time scales.

- **Atomistic**
  - Experimental methodology testing
  - Processes and mechanism identification
  - Calculations feed into mesoscale model parameterization
- **Mesoscale**
  - Crystal plasticity model with dislocation kink-pair theory integrates microstructure into models
  - Calculations feed into continuum model parameterization
- **Continuum**
  - Macroscopic scale simulation for experimental analysis

Molecular dynamics approach

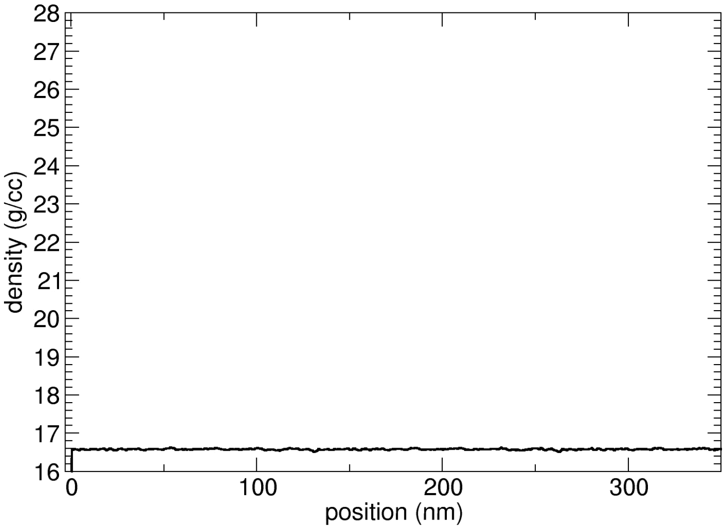


- **Strengths of MD method**
  - *Controlled material structures, i.e. grains, defects*
  - *Repeatable loading profiles at rates, from 10^{11} to 10^{8}*
  - *Full stress state throughout the sample*
  - ***However**, we do not achieve overlap in strain rate, nor microstructure.*

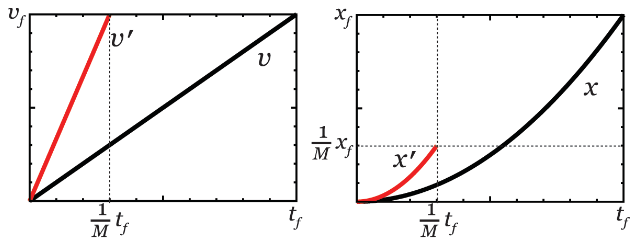
Several MD studies of shock, plasticity and dislocations

Ravelo, et al., PRB, 88 134101 (2013)
Tang, Bringa, Meyers, Mater. Sci. Eng. 580 414 (2013) &
Tramontina, et al., High Energy Density Phys, 10 (2014)

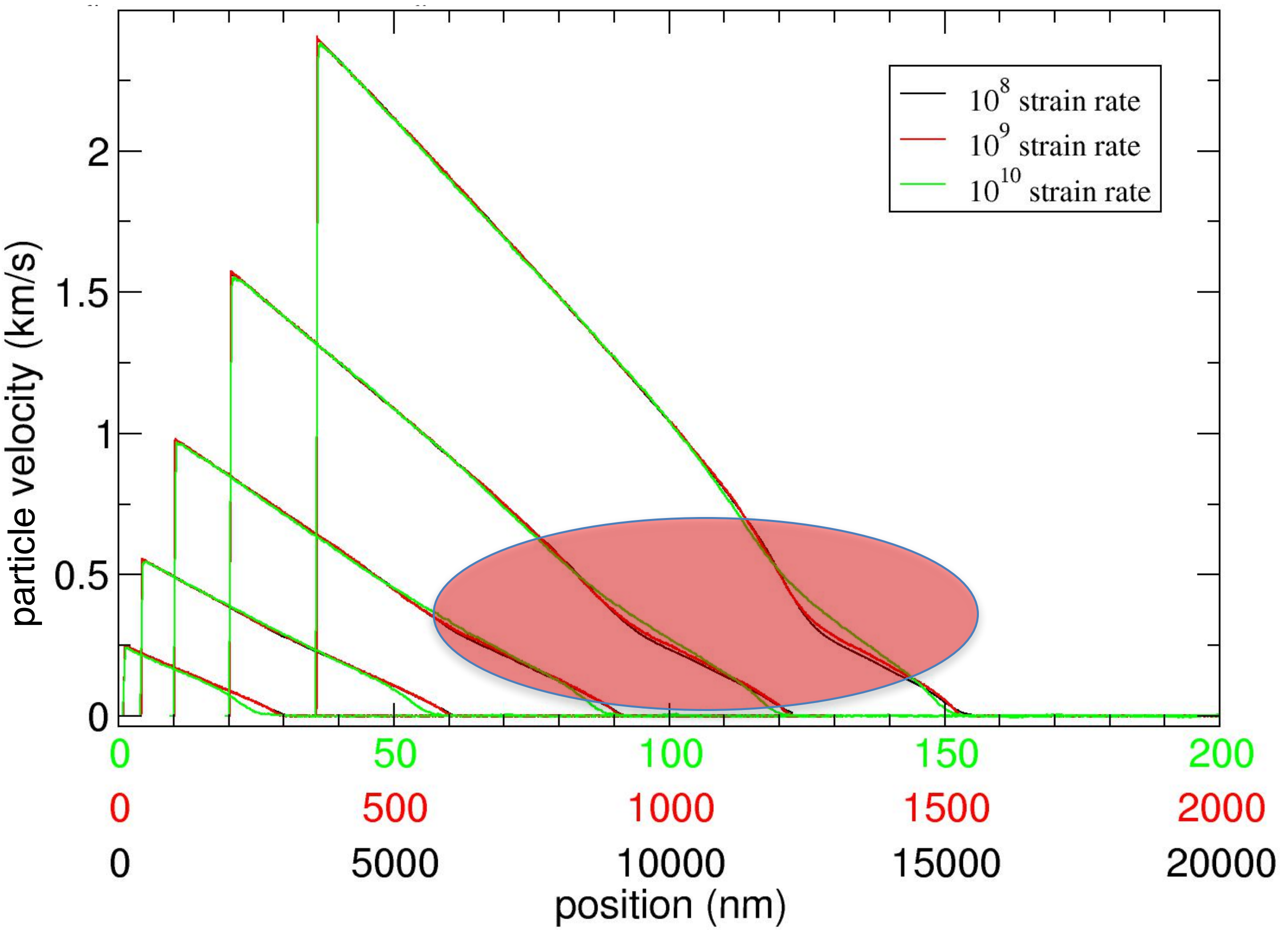
- **Classical molecular dynamics**
  - *Ta1 EAM potential by Ravelo was fit to isothermal EOS and verified against Hugoniot data*
    - captures twinning and plastic flow.
  - *Ramp wave modeled with accelerating infinite-mass piston with nonlinear profile $v_p = x/a + (x/a)^3$*
- **System size and grain structure**
  - *20 x 20 x 131 nm nanograin polycrystalline unit cell replicated in z to 20 μm and 350 million atoms*
  - *Two grain sizes of 5-10 nm and 8-20 nm*



Scaled ramp profiles & strain-rate sensitivity



Using scaling arguments, we can compare strain rate response.
Lane, Foiles, Lin, Brown, Phys. Rev. B, 94, 064301 (2016)



All ramp waves are driven nonlinearly from 0 to 2.4 km/s, giving peak pressures of 250 GPa.

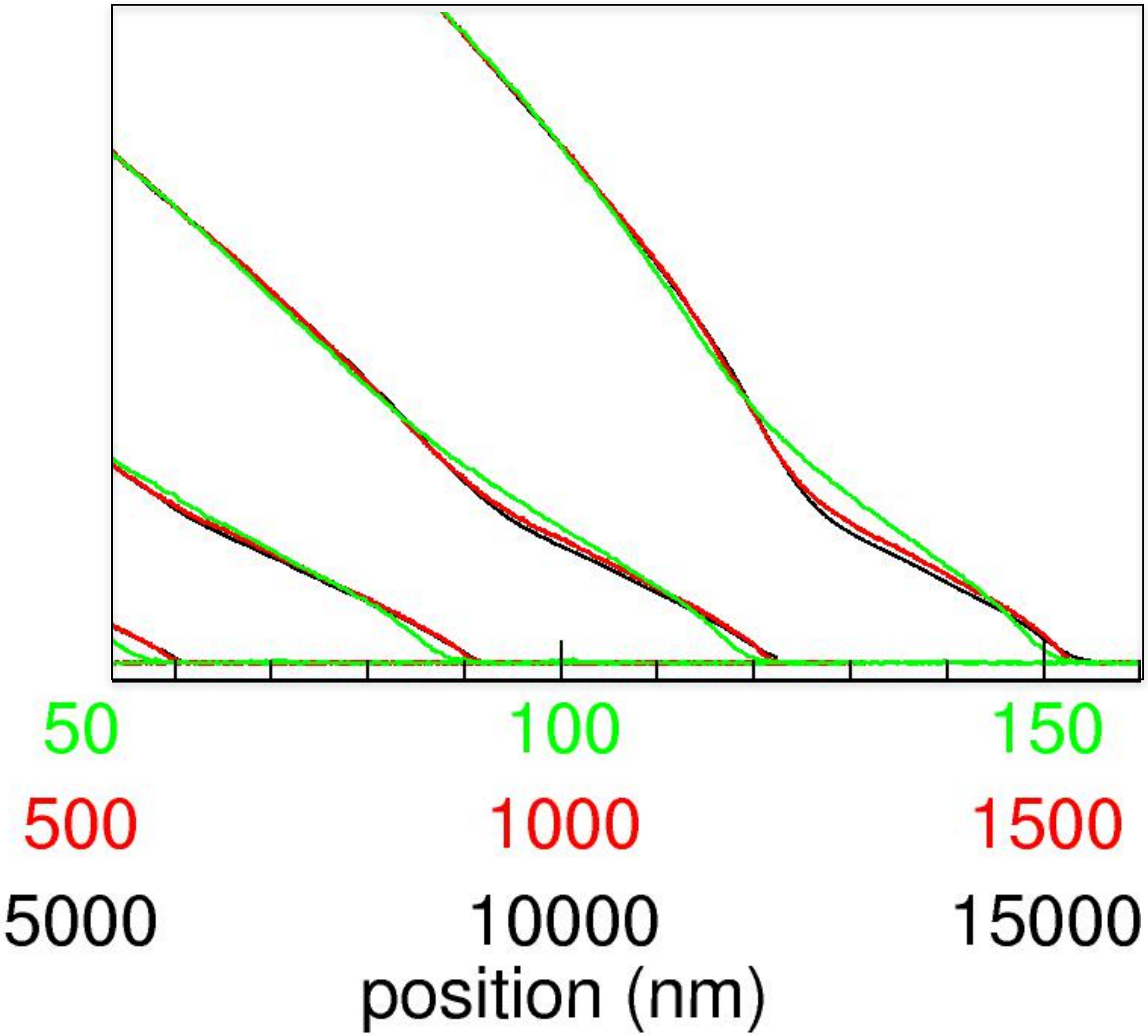
10^{10} 1/s strain rate
Rises over 40 ps
150 nm & 2.5 million atoms

10^9 1/s strain rate
Rises over 400 ps
1.5 µm & 25 million atoms

10^8 1/s strain rate
Rises over 4 ns
15 µm & 350 million atoms

Matthew Lane - jlane@sandia.gov

Precursor dependence on strain rate



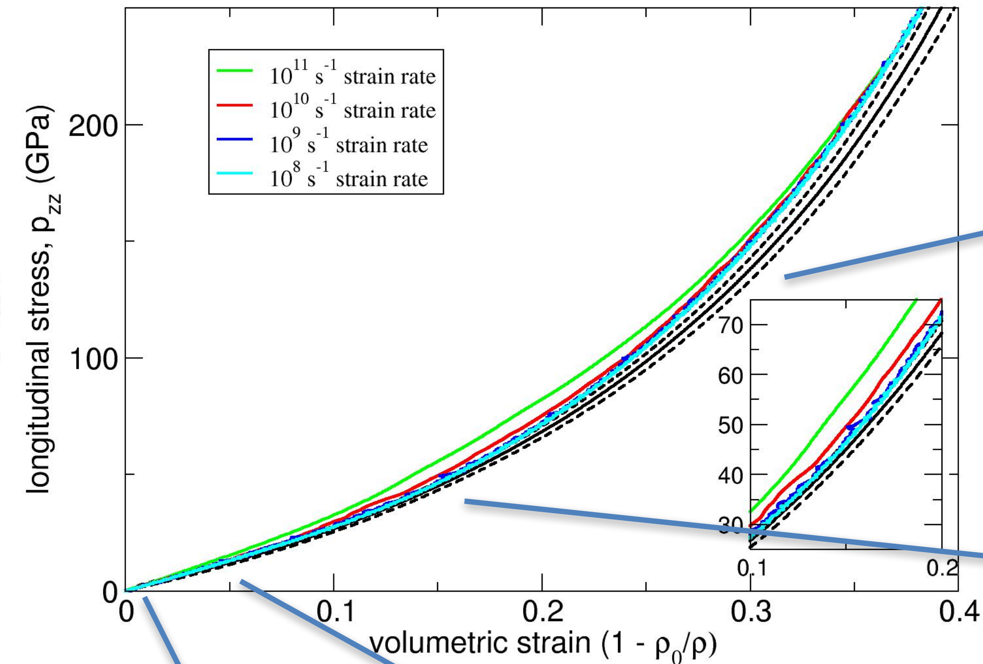
Overlaying scaled profiles reveals where the wave profiles are dependent on strain-rate.

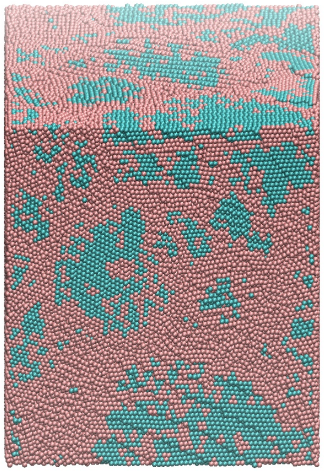
Elastic precursor and precursor decay depends significantly on strain rates.

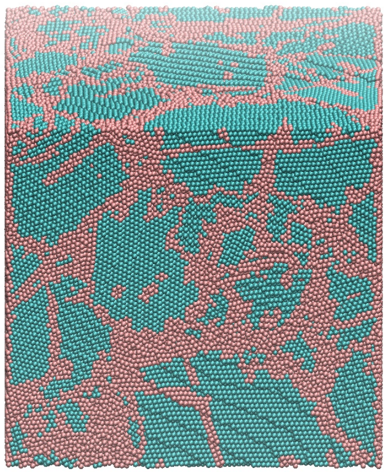
High pressure portions of the waves are only weakly dependent on loading rate.

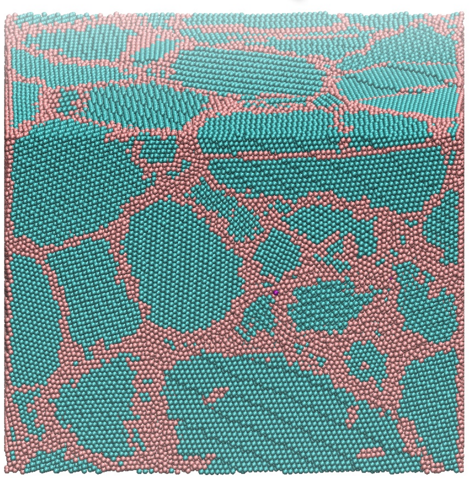
Comparison with experiment

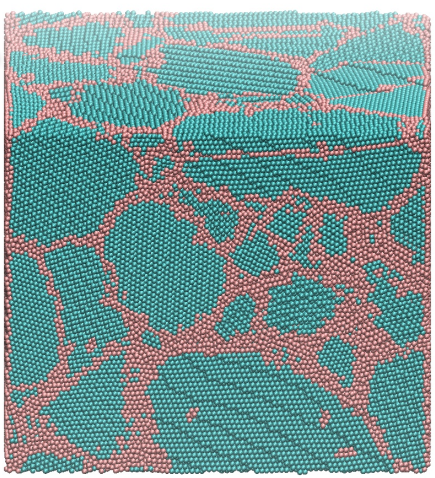
Davis et al. JAP, 116 204903 (2014)







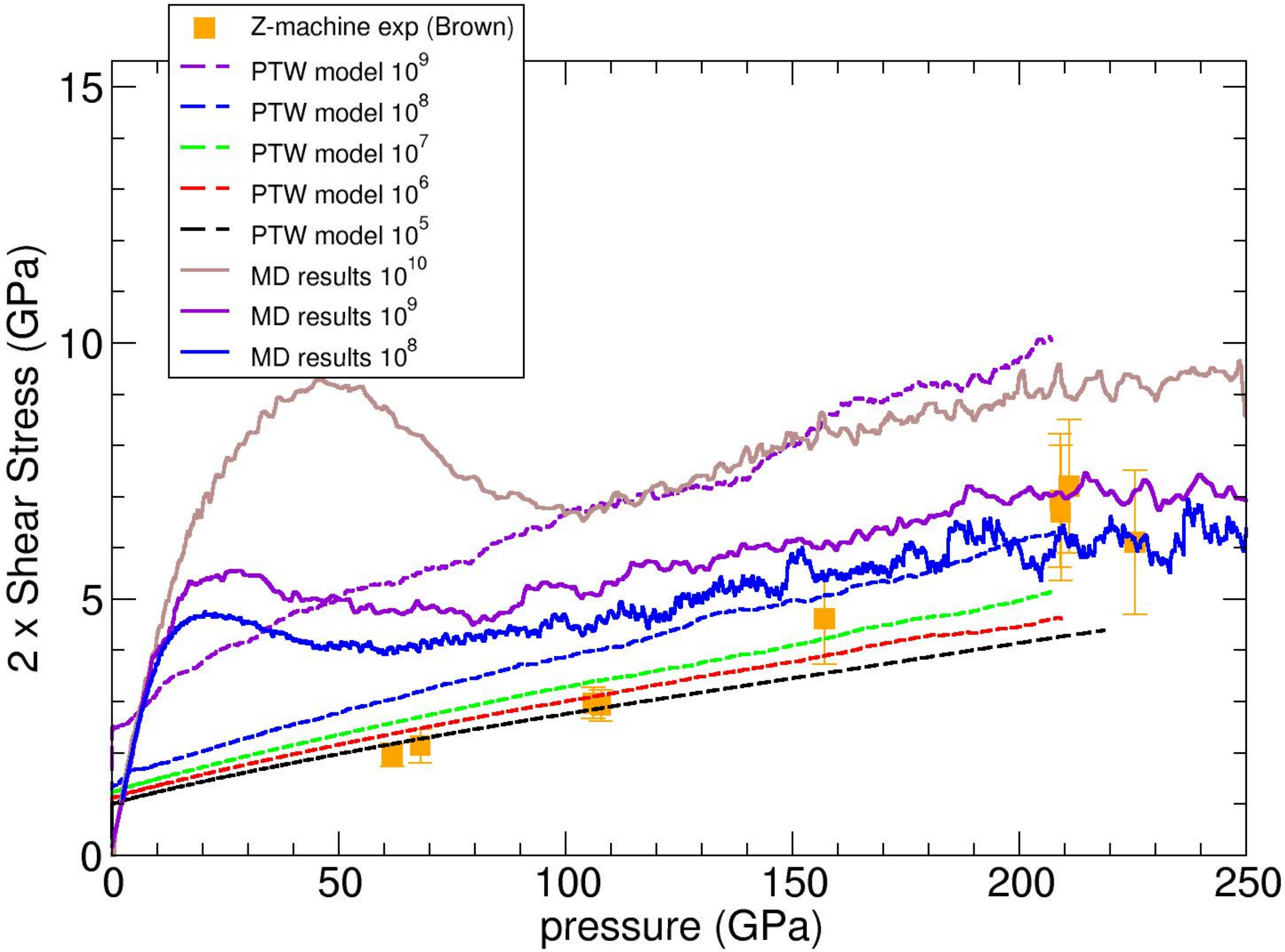




Inverse Hall-Petch response dominated by grain boundary sliding

Consistent with *Tang, Bringa, Meyers, Mater. Sci Eng. A,* ***580*** *(2013)*

Extraction of strength

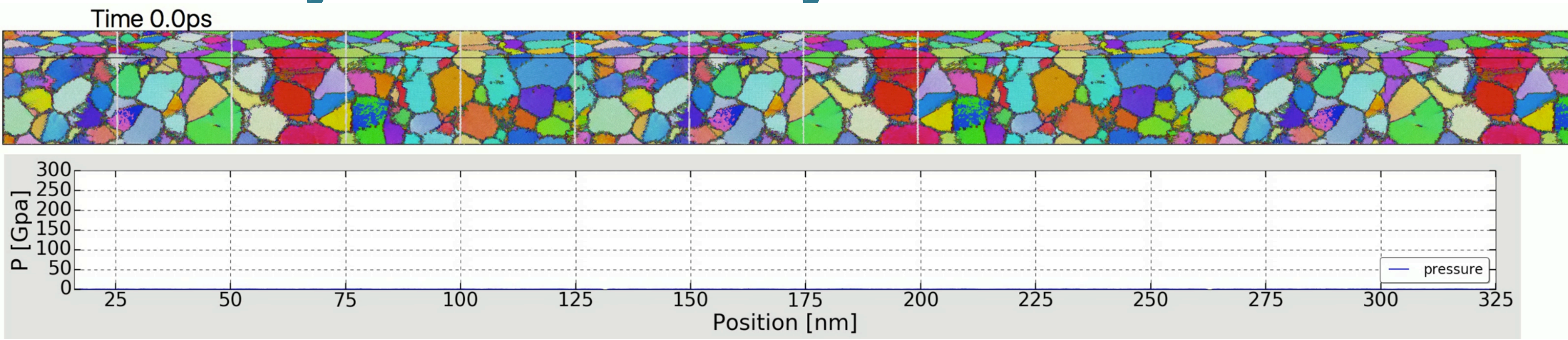


Exaggerated strength is seen below 100 GPa in the elastic precursor, especially at high strain rates. This is likely due to suppressed dislocation activity in nano size grains.

Relatively good agreement with pressure dependence of the PTW model above 100 Gpa, especially at lower strain rates.

PTW model – Preston, Tonks, Wallace, JAP, 93 211 (2003)

Nanocrystalline Plasticity



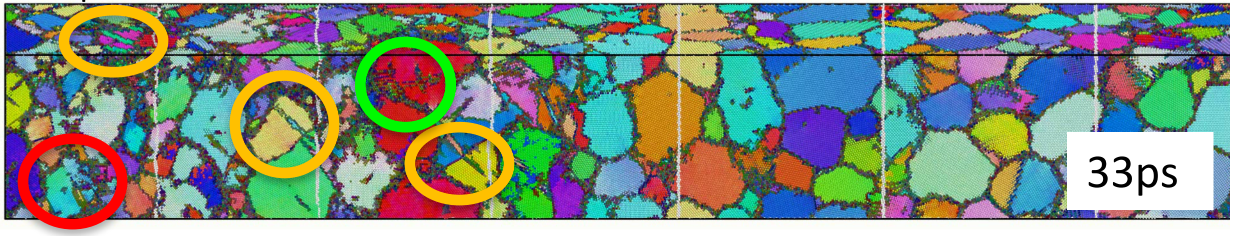
Twinning:

Stacking faults & dislocations:

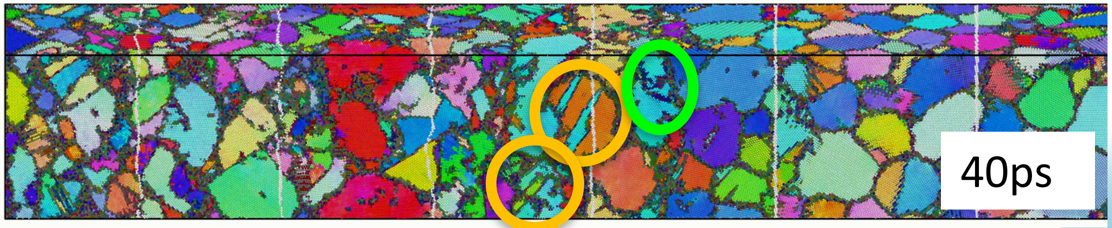
Grain growth:

- Compression:
  - Stacking faults and dislocations emitted from GBs.
  - Some stacking faults grow to become twins.
  - Grain growth is observed.
- Release:
  - Most compression twins disappear and new release twins form and grow.
  - Significant grain reorientation is observed.

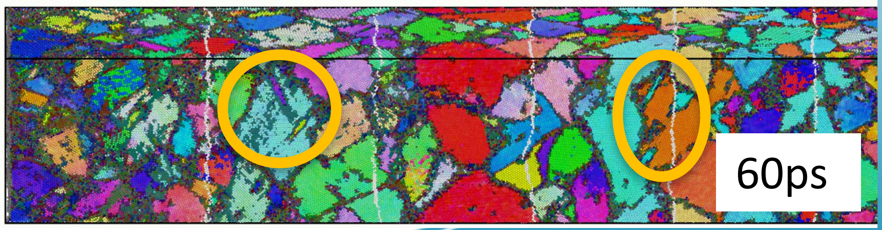
compression



compression



release



Lagrangian Wave Analysis

- X is the Lagrangian coordinate.
- For isentropic flow of simple waves, the Lagrangian wave speed "c" can be calculated using the particle velocity histories at different locations.

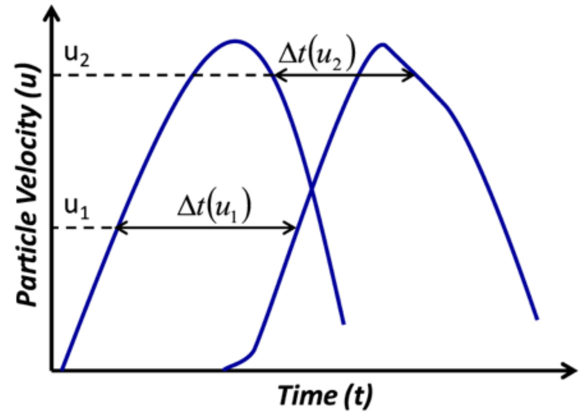
$$C_u = c_L(u_p) = (\partial X/\partial t)_u = \frac{\Delta X}{\Delta t}_u$$

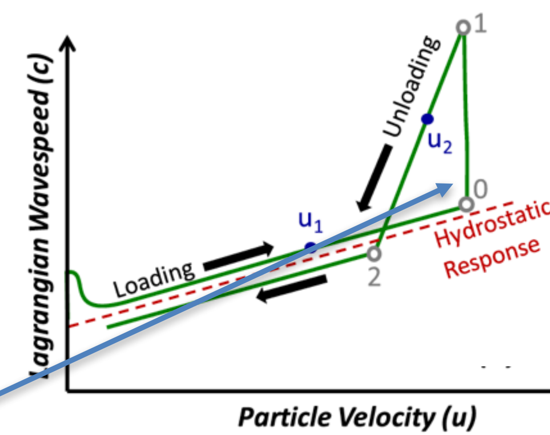
- The Lagrangian wavespeed can then be used to determine changes in the shear stress at pressure.

$$\sigma_x = \bar{\sigma} + (4/3)\tau \rightarrow \frac{d\sigma_x}{d\varepsilon} = \frac{d\bar{\sigma}}{d\varepsilon} + \frac{4}{3}\frac{d\tau}{d\varepsilon}$$

$$d\varepsilon = \frac{du}{c(u)} \rightarrow \rho_0 c^2 = \frac{d\sigma_x}{d\varepsilon} \leftarrow d\sigma_x = \rho_0 c(u) du$$

$$\tau(u_1) - \tau(u_2) = \frac{3}{4}\rho_0 \int_{u_2}^{u_1} [c^2(u) - c_B^2(u)] \frac{du}{c(u)}$$





Brown, et al., J. Appl. Phys. 114, 223518 (2013).

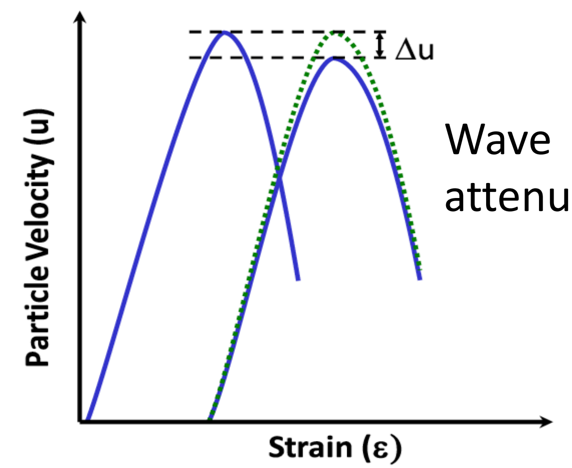
Calculation of Dynamic Properties

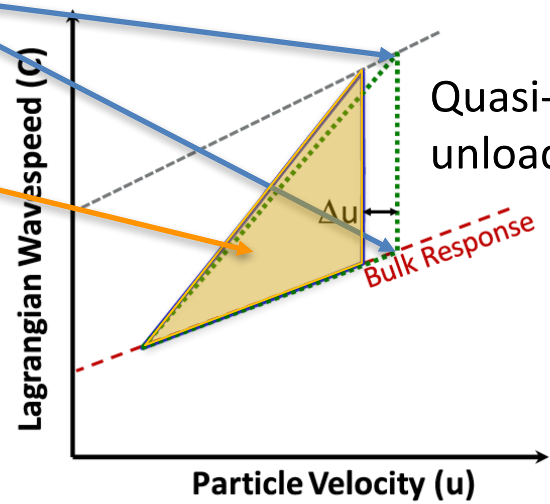
$$\tau(u_1) - \tau(u_2) = \frac{3}{4}\rho_0 \int_{u_2}^{u_1} [c^2(u) - c_B^2(u)] \frac{du}{c(u)}$$

$$C_L = C_B \sqrt{1 + \left({}^4/_3\right)\left({}^{\partial\tau}/_{\partial P}\right)}$$

$$G = \rho_0(1 - \varepsilon_{max} - \varepsilon_{attenuation}) \sqrt{\frac{3}{4}(c_L^2 - c_B^2)}$$

$$Y = \int_{\varepsilon_{trans}}^{\varepsilon_{max}} G_{eff}\, d\varepsilon$$





Attenuation of the peak particle velocity or pressure occurs when the rarefaction wave overtakes the compression wave.

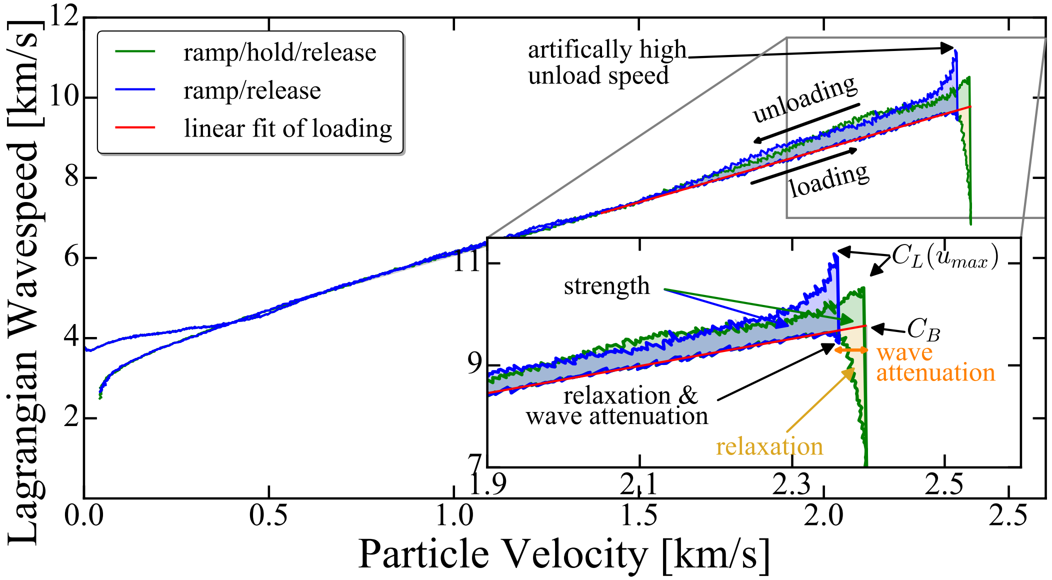
$$K = \rho_0(1 - \varepsilon_{max} - \varepsilon_{atten})C_b^2 \qquad \nu = \frac{3C_b^2 - C_l^2}{3C_b^2 + C_l^2}$$

Brown, et al., J. Appl. Phys. 114, 223518 (2013).

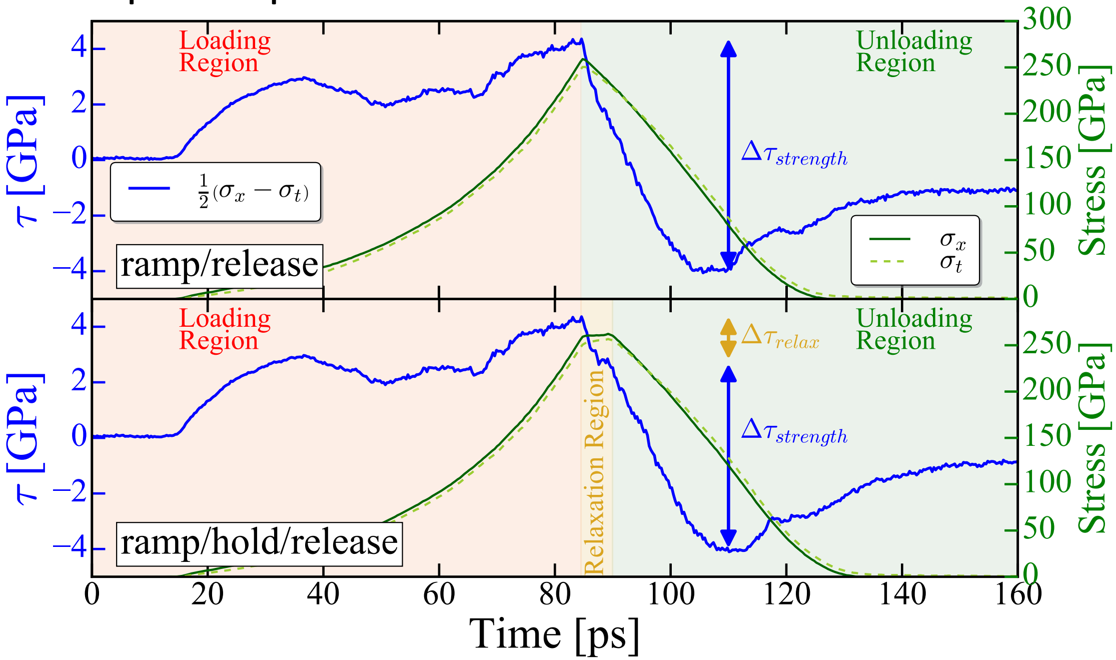
Shear Stress Dependence

Idealized elastic-plastic theory assumes the shear stress τ, is the maximum critical shear stress (τ_C) of the material, which is normally a constant.

In reality τ_C during ramp compression loading is dependent on the temperature, hydrostatic pressure, loading rate, microstructure, and path history.



Time profiles of pressure tensor and shear stress.

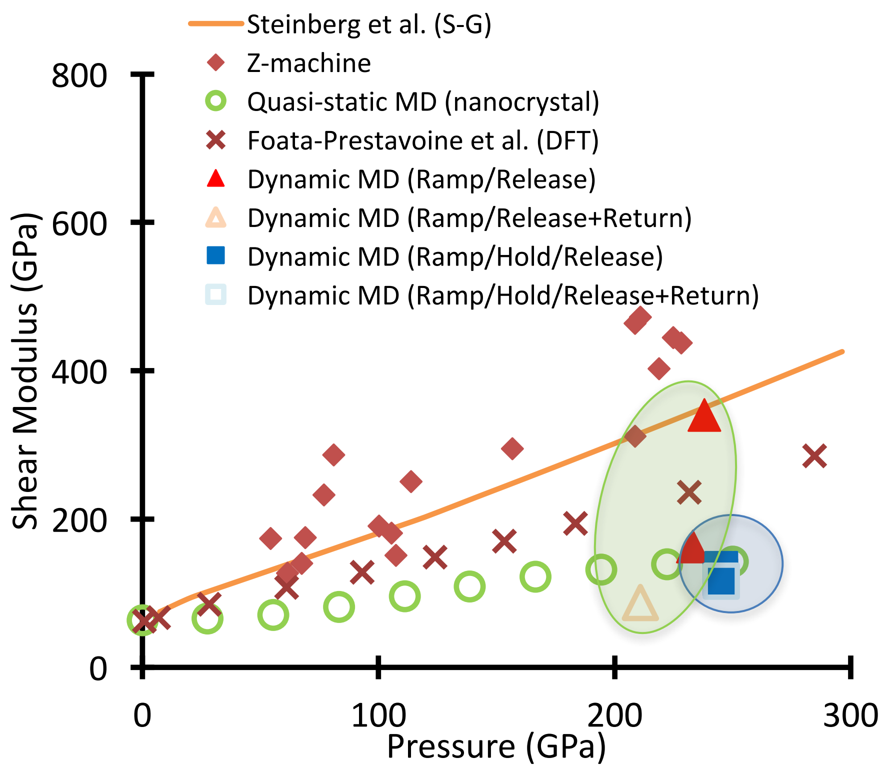


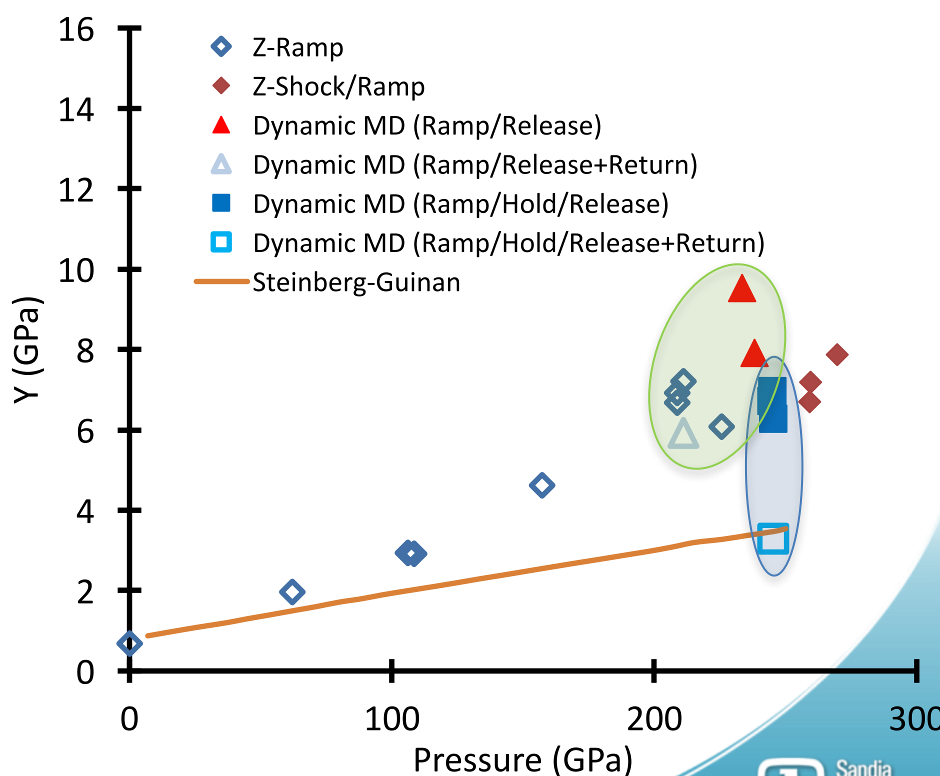
Ramp/hold/release profile in the hold region, showing relaxation via additional plasticity.

This illustrates that the critical resolved shear stress is dependent on the strain rate, and causes a Lagrangian wavespeed slowing effect in the compression wave near peak particle velocities.

Updated Dynamic Results

- **Attenuation and Strain Rate:** effects combined tend to cause an increase in the reported shear modulus, and a slight increase the reported strength.
- The ramp/hold/release dynamic MD results agree with the quasi-static MD, validating the analysis methodology, when strain rate effects are removed.





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Atomistic progress review

- We've studied dynamic ramp wave response in nanocrystalline tantalum at 10^{11} to 10^{8} 1/s strain rates with molecular dynamics and ramp profile scaling analysis.

- Reasonable agreement in stress-strain response with lower-rate experiments (Davis, et al.)
    - Lower strain rate brings better comparison, especially at strain below 0.2
    - Over-represented elastic response produces a more robust precursor which may drive up longitudinal stress at high strains.

- MD validates the self-consistent Lagrangian analysis and identifies the need for improved experiments to improve dynamic measurement reliability.

Mesoscale modeling motivation

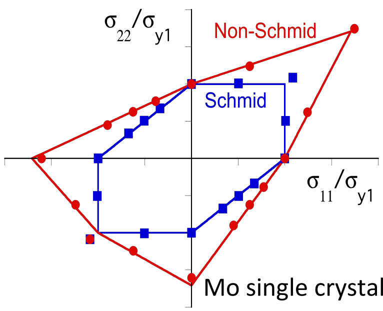
- Sandia has interest in Ta mechanical properties in high strain rate environments, especially rate and microstructure dependent response.
- **Most conventional strength models are largely empirical, and can't be extrapolated outside the calibration space.**
- **Next-generation strength models need more physical basis.** We can build on the extensive work and experience that the physics labs have created in understanding Ta properties.
- **We up-scale from single crystal plasticity, through the polycrystal scale, and to the macro-scale for a validated, predictive multi-scale strategy.**
- **How do can we predictively model Ta mechanical properties in the regimes of interest to the engineering labs?**
  - The strength of a BCC metal is governed primarily by dislocation plasticity (in abnormal environments...).
  - Body-centered cubic metals (α-Fe, Mo, Ni, Ta, T-111, V, W) deform by the slip of screw dislocations.
  - Screw dislocations move by the formation of "kink pairs" that "unzip" the dislocation line.

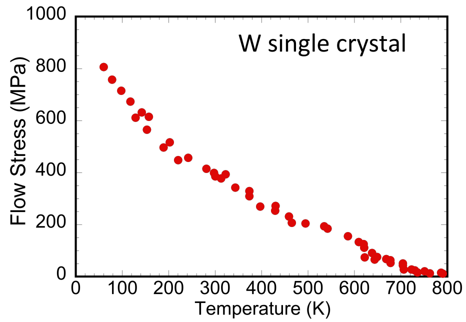
Matthew Lane - jlane@sandia.gov

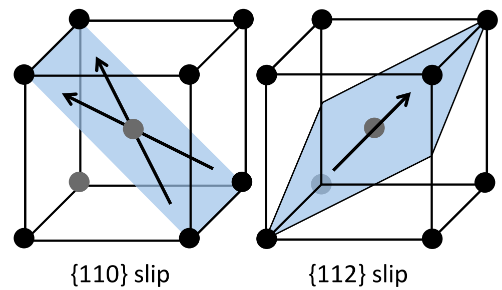
Introduction

❖ Need *physically-based* model for BCC metals

- **Complex response compared to FCC**
  - *Non-Schmid effects, large temp. & rate dep. flow behavior,* ambiguity of slip systems,



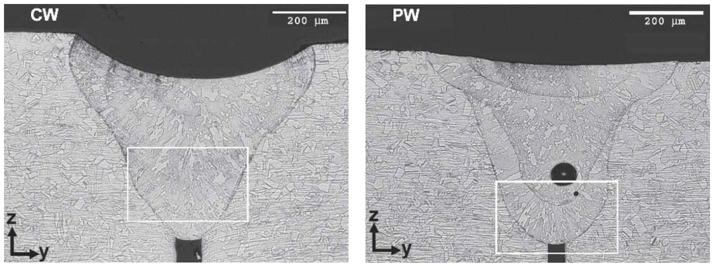




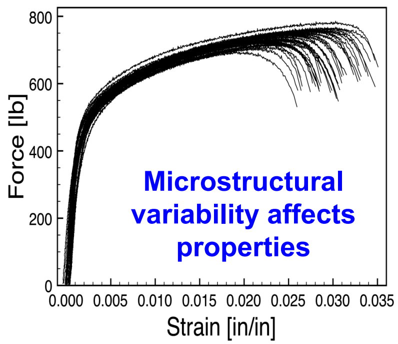
- **Most BCC models are phenomenological, fit from polycrystals**

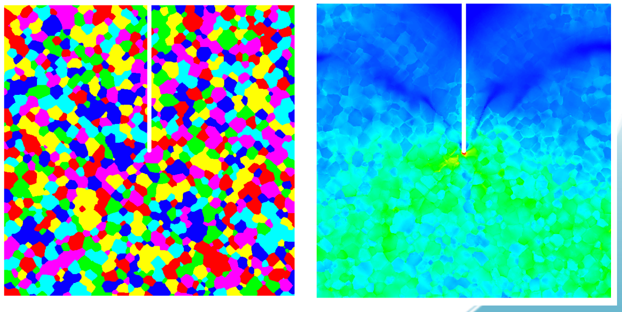
❖ Need capability to include *microstructural variability* in design

- **Connecting microstructural variability to stochastic performance**



Microstructural details vary among 304L stainless steel weldments





CP-FEM simulations

Matthew Lane - jlane@sandia.gov

Ta crystal plasticity for low-rate strength model

Modified dislocation kink-pair theory:

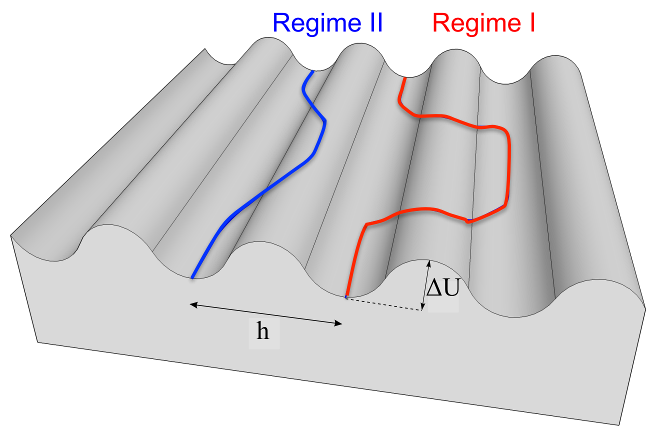
Temperature, strain rate & pressure dependence

Hojun Lim

$$\underbrace{\tau(T,\dot{\gamma})}_{} = \underbrace{\tau^{*}(T,\dot{\gamma})}_{\text{Thermal}} + \underbrace{\tau_{obs}}_{\text{Athermal}}$$

In FCC metals, $\tau^{*} \approx 0$

In BCC metals, $\tau^{*} >> 0 \quad (T << T_c)$



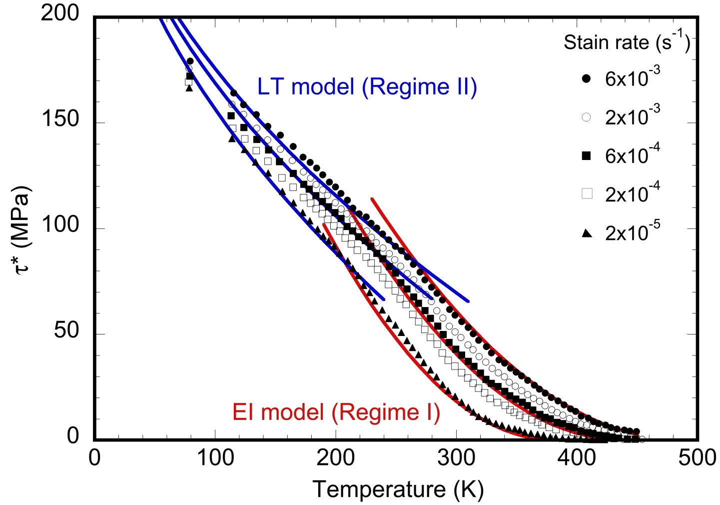
Elastic Interaction Model (Regime I)

$$\tau^{*}_{EI} = \frac{\mu}{\mu_0}\tau^{0}_{EI}\left(1 - \frac{\mu_0}{\mu}\frac{T}{T^{0}_{c}(\dot{\gamma})}\right)^{2}$$

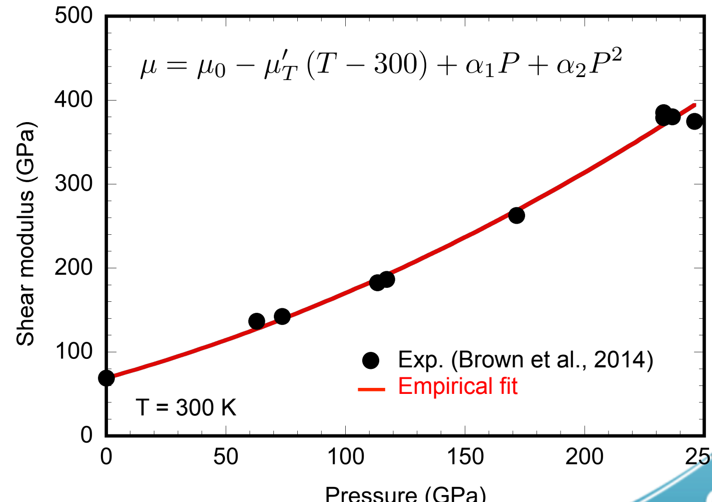
Line Tension Model (Regime II)

$$\tau^{*}_{LT} = \frac{\mu}{\mu_0}\tau^{0}_{LT}\left(1 - \left(\frac{\mu_0}{\mu}\frac{T}{T^{0}_{c}(\dot{\gamma})}\right)^{1/2}\right)$$

Temperature and strain rate dependence



Pressure dependence



Matthew Lane - jlane@sandia.gov

Analytical model for polycrystalline Ta

Ta strength model incorporating temperature, strain rate and pressure

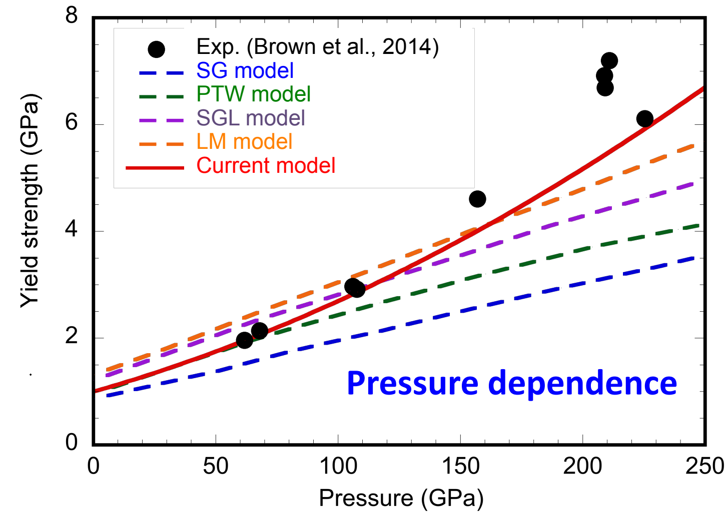
$$\tau = \min\left(\tau^*_{EI}, \tau^*_{LT}\right) + \tau_{obs}$$

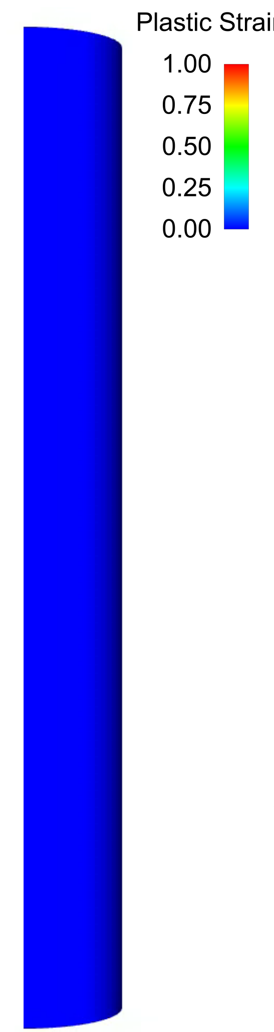
$$\sigma = \bar{M}\tau$$

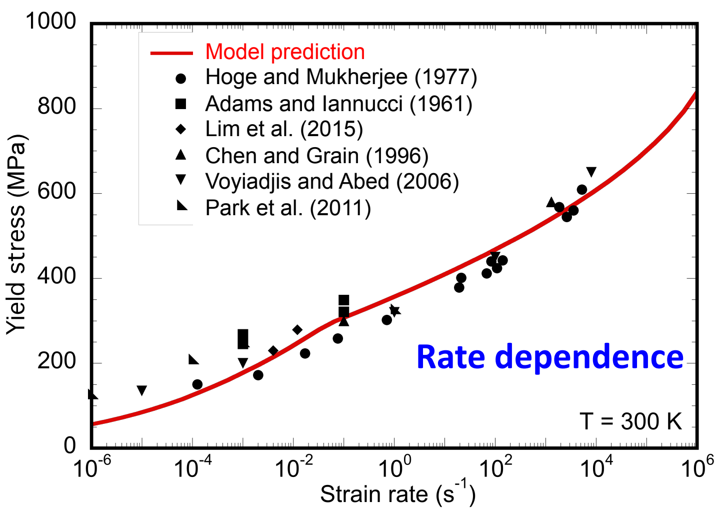
σ : Tensile stress of polycrystal

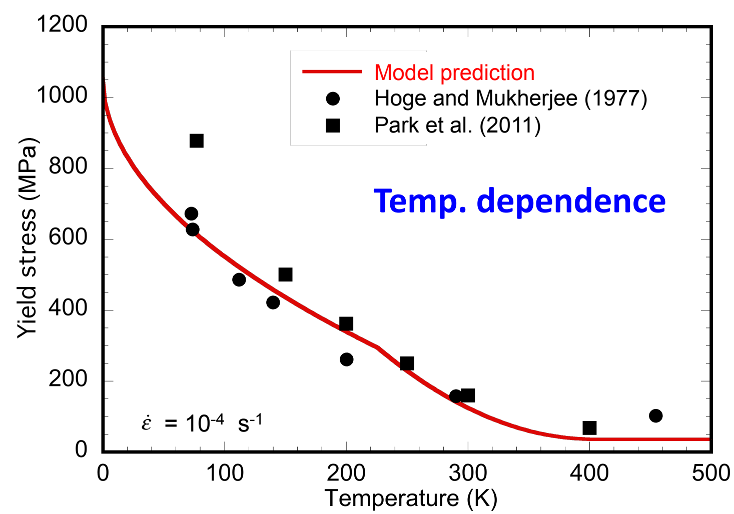
τ : Shear stress of single crystal

$\bar{M}$: Taylor factor (~3.07 for BCC)







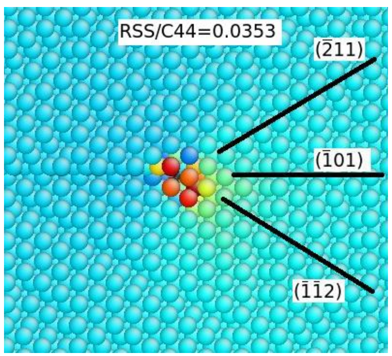


Matthew Lane - jlane@sandia.gov

Crystal Plasticity FEA Method

- Crystal plasticity = Grain-level (mesoscale) approach to materials modeling using multiscale strategies
- Explicitly model discrete grains and slip systems (anisotropy, texture evolution,…)

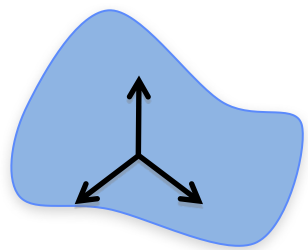
Atomic phenomenology: Fundamental deformation mechanisms



Yield criterion:

$$\sigma_{cr}^{app}[a_0\mathbf{m}^{(s)}\mathbf{n}^{(s)} + a_1\mathbf{m}^{(s)}\mathbf{n}^{(s')} + a_2\left(\mathbf{n}^{(s)} \times \mathbf{m}^{(s)}\right)\mathbf{n}^{(s)} + a_3\left(\mathbf{n}^{(s)} \times \mathbf{m}^{(s)}\right)\mathbf{n}^{(s')}] = \tau_{cr}$$

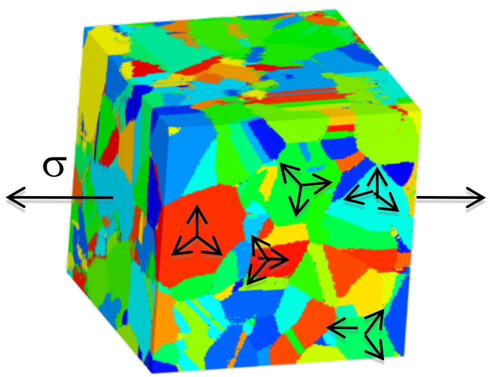
Single crystal plasticity: Deformation of one, isolated crystal



Constitutive law:

$$\dot{\gamma}^{(s)} = \frac{\tau^{(s)}}{\tau_{cr}}\left|\frac{\tau^{(s)}}{\tau_{cr}}\right|^{\frac{1}{m}-1}$$

Polycrystal plasticity: Assemble single crystals into polycrystalline ensemble



Prediction of collective deformation behavior.

BCC Crystal Plasticity Framework

- FEM code developed at Sandia National Laboratories (JAS-3D)
- 24 {110}<111> slip systems
- Slip rate: $\dot{\gamma}^{\alpha} = \dot{\gamma}_0^{\alpha} \left(\frac{\tau^{\alpha}}{g^{\alpha}} \right)^{1/m}$ (Hutchinson, 1976)
- Slip resistance: $g^{\alpha} = \min\left(\tau_{EI}^{*\alpha}, \tau_{LT}^{*\alpha}\right) + \tau_{obs}^{\alpha}$

  τ_{obs}^{α} → Obstacle stress

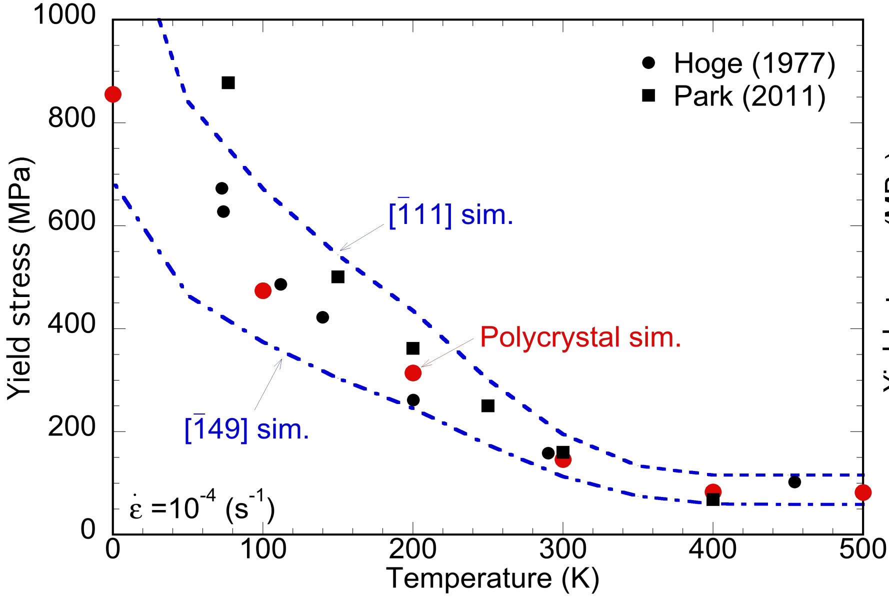
  $\min\left(\tau_{EI}^{*\alpha}, \tau_{LT}^{*\alpha}\right)$ → Lattice friction
- Obstacle stress: $\tau_{obs}^{\alpha} = A\mu b \sqrt{\sum_{\beta=1}^{NS} \rho^{\beta}}$ (Taylor, 1934)

$$\dot{\rho}^{\alpha} = \left(\kappa_1 \sqrt{\sum_{\beta=1}^{NS} \rho^{\beta}} - \kappa_2 \rho^{\alpha} \right) \cdot \left| \dot{\gamma}^{\alpha} \right|$$ (Kocks, 1976)

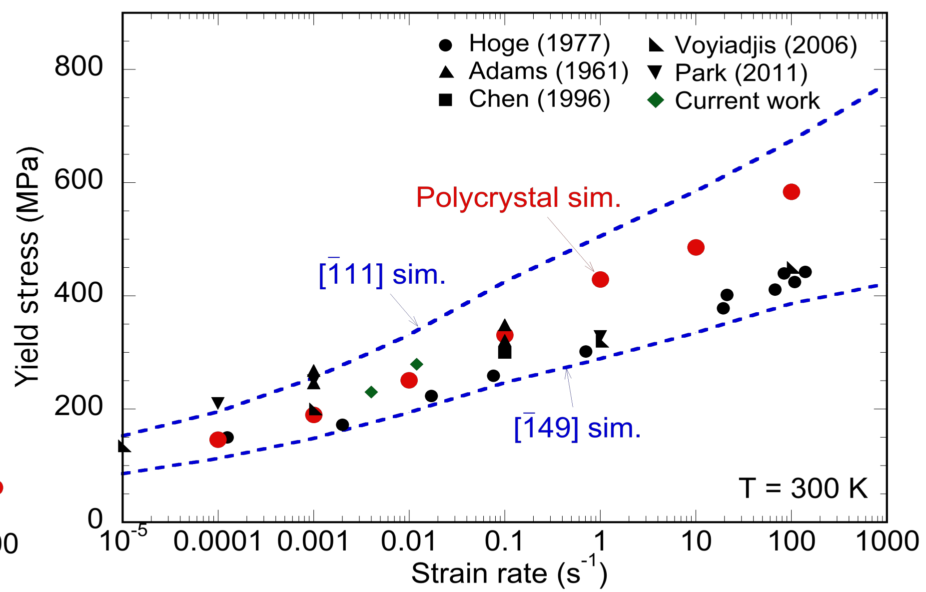
Matthew Lane - jlane@sandia.gov

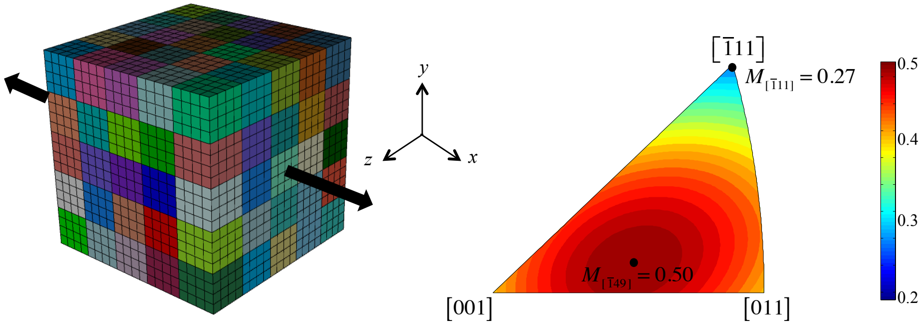
Temperature and Strain Rate Dependence

Temperature dependence



Strain rate dependence





Measured yield stresses of BCC polycrystals lie between the bounds predicted by CP-FEM models on extreme single crystal orientation.

ALEGRA materials library for Tantalum

Model	Source	Rates (s^{-1})
JC	AFRL,1983	10^{-2} - 4×10^{2}
ZA	NSWC,1990	10^{-4} - 5×10^{3}
MTS	LANL, 1996	10^{-3} - 3×10^{3}
SGL	LLNL, 1989	10^{-4} - 10^{6}
PTW	LANL, 2003	10^{-3} - 10^{12}
KP	SNL, 2014	10^{-5} – 10^{5} ?

$$\sigma_y^{JC} = A\left(1 + C\ln\dot{\varepsilon}\right)\left(1 - T^{*m}\right)$$

$$\sigma_y^{ZA} = C_0 + C_1\exp\left(-C_3T + C_4T\ln\dot{\varepsilon}\right)$$

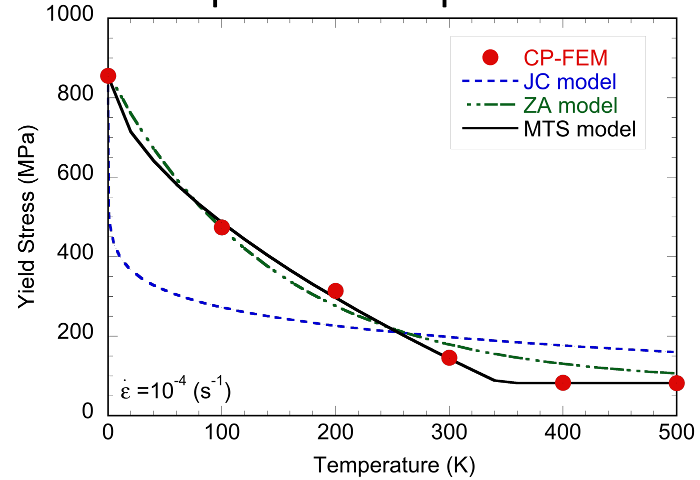
$$\sigma_y^{MTS} = \sigma_0 + \hat{\sigma}\left(1 - \left(-\frac{k_B}{G_0}T\ln\frac{\dot{\epsilon}}{\dot{\epsilon}_0}\right)^{1/q}\right)^{1/p}$$

$$\sigma_y^{SGL} = \frac{\mu(P,T)}{\mu_0}\left(\sigma_T(\dot{\epsilon},T) + \sigma_A f(\epsilon)\right) \qquad \dot{\epsilon}_p = \left\{\frac{1}{C_1}\exp\left[\frac{2U_K}{kT}\left(1 - \frac{Y_T}{Y_P}\right)^2\right] + \frac{C_2}{Y_T}\right\}$$

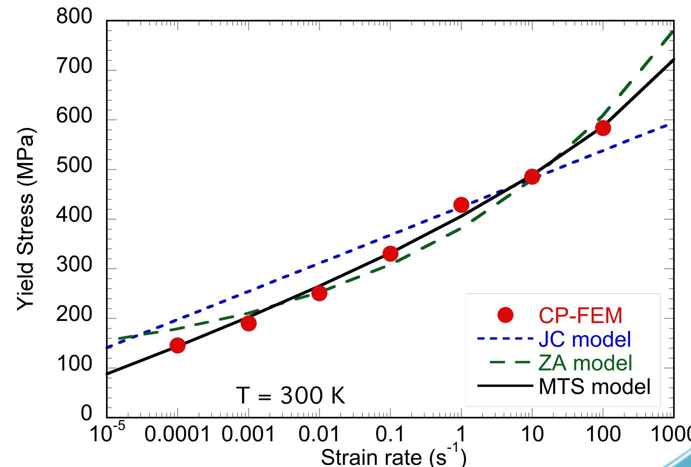
$$\sigma_y^{PTW} = \hat{\tau}_s + \frac{1}{p}(s_0 - \hat{\tau}_y)\ln\left[1 - \left[1 - \exp\left(-p\frac{\hat{\tau}_s - \hat{\tau}_y}{s_0 - \hat{\tau}_y}\right)\right] \times \exp\left\{-\frac{p\theta\psi}{(s_0 - \hat{\tau}_y)\left[\exp\left(p\frac{\hat{\tau}_s - \hat{\tau}_y}{s_0 - \hat{\tau}_y}\right) - 1\right]}\right\}\right]$$

$$\sigma_y^{KP} = M\left(\min\left(\tau_{EI}^*, \tau_{LT}^*\right) + \bar{\tau}\right)$$

Temperature dependence



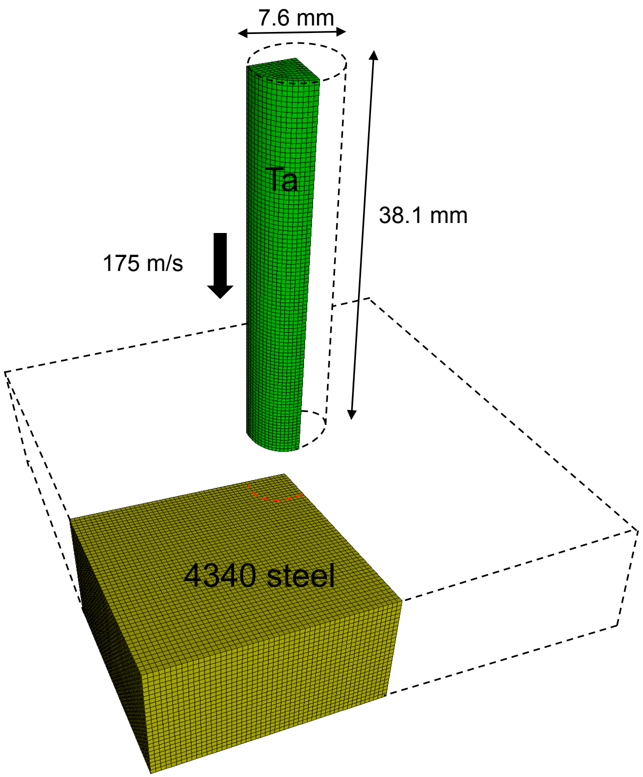
Strain rate dependence

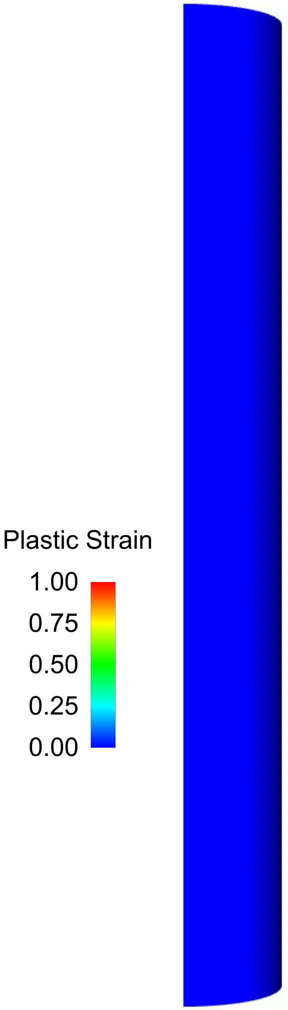


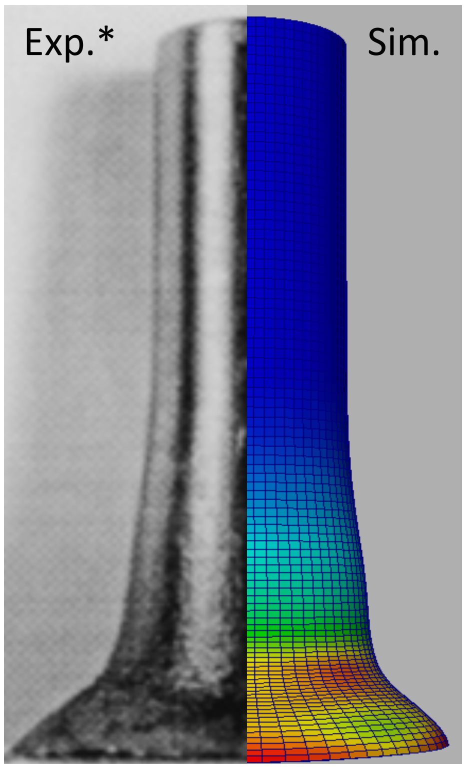
MTS model most accurately reproduces temperature & rate dependent polycrystalline behavior

High-rate dynamic simulations

Taylor cylinder impact test





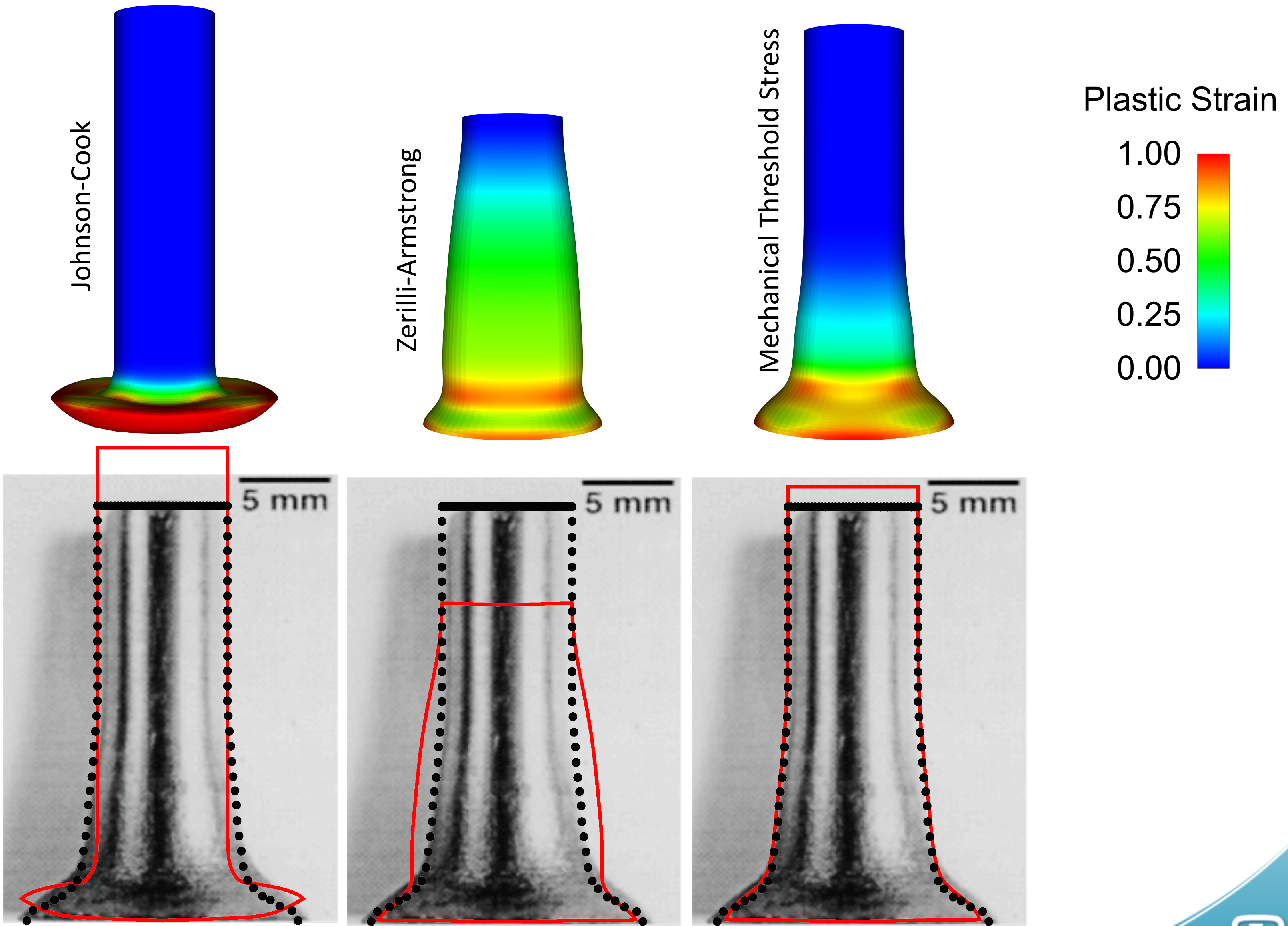


Deformed geometry

- ALEGRA solid dynamics code (Sandia)
- Kerley Mie-Grüneisen equation of state
- Strength models:
  - Kink-pair (KP) model
  - Johnson-Cook (JC) model
  - Zerilli-Armstrong (ZA) model

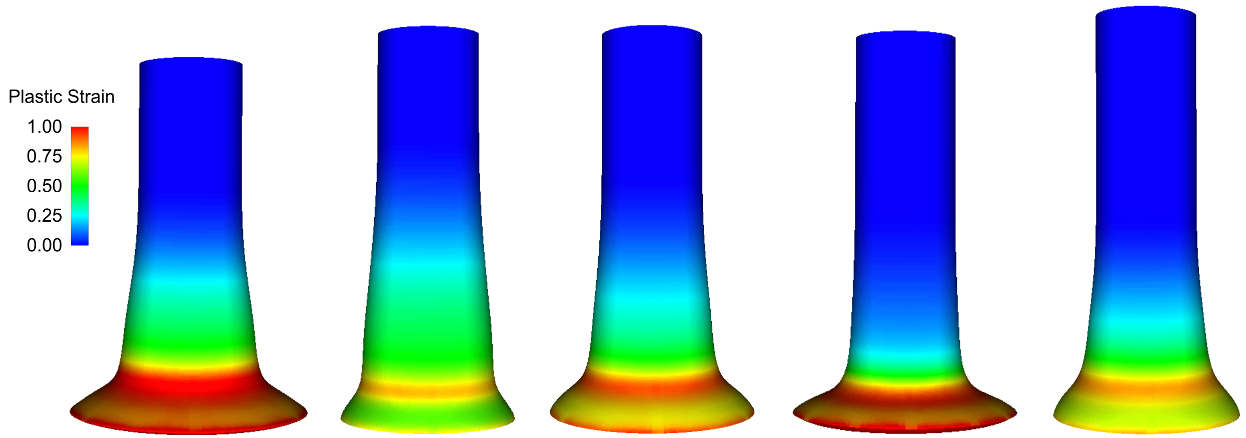
* Maudline et al., IJP (1999)

Taylor Simulation Results (ALEGRA)

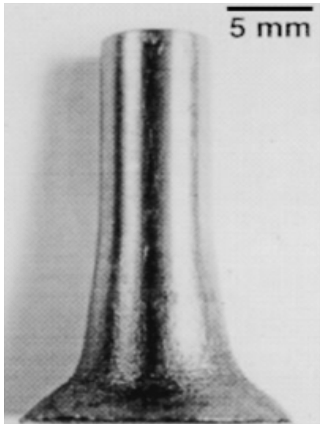


(Maudlin 1999)

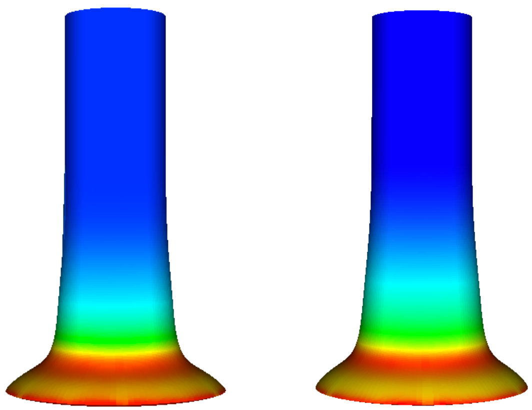
Simulation of Taylor impact tests



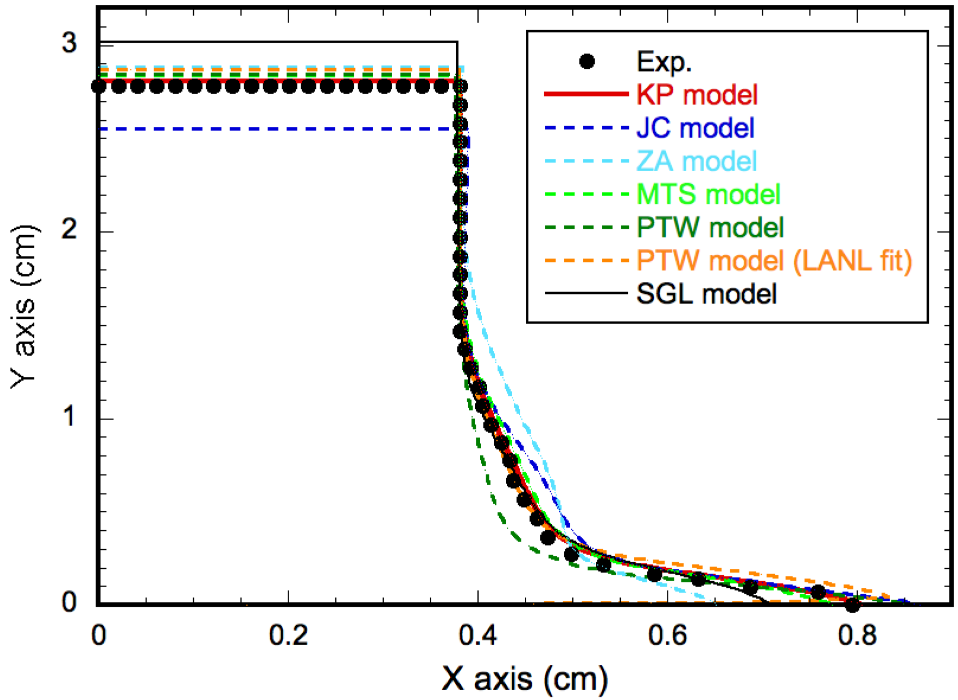
JC model | ZA model | MTS model | PTW model | SGL model



Experiment



PTW model (LANL fit)* | KP model



*Strength/EOS fit to LANL parameterization to STARCK Ta

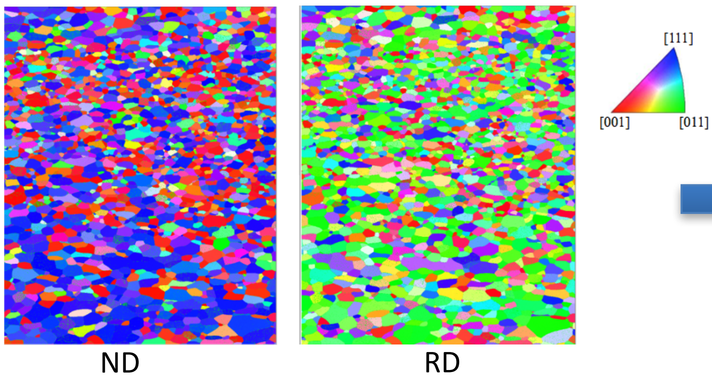
Mesoscale and continuum progress review

- Developed **temperature**, strain rate and pressure dependent flow rule based on dislocation kink-pair theory for Ta.
- **CP-FEM predictions showed good agreement with experiments.**
- **Developed conformal, hexahedral finite element meshing technology for three-dimensional polycrystalline microstructures**

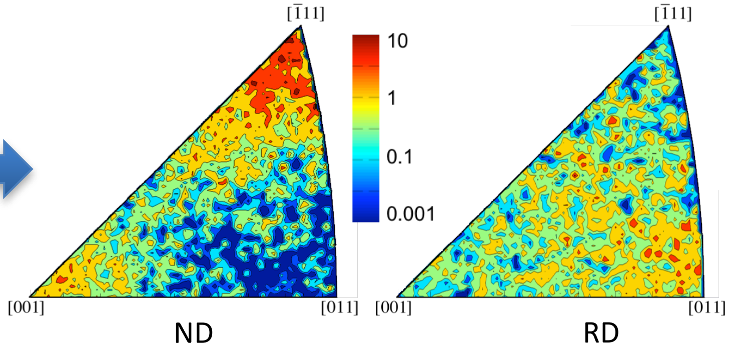
- **Proposed computational method provides a convenient and direct link from the fundamental dislocation physics to the macro-scale plastic deformation of polycrystalline tantalum.**

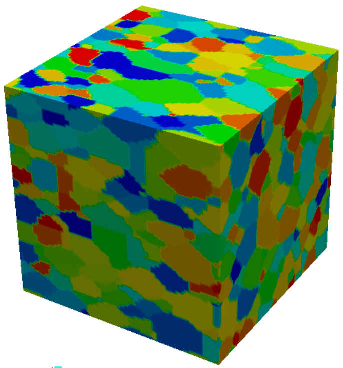
Developing Ta anisotropic yield model using EBSD and mesoscale model

Texture measurement (EBSD)

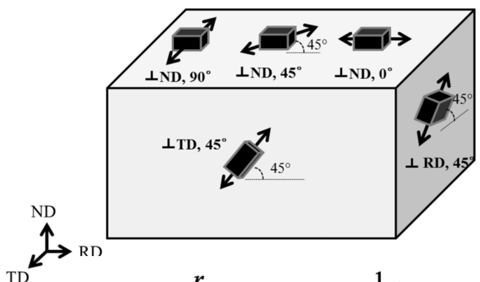


Crystal plasticity finite element model





Developing continuum anisotropic yield model



$$\phi = F\left(\sigma_{yy}-\sigma_{zz}\right)^2 + G\left(\sigma_{zz}-\sigma_{xx}\right)^2 + H\left(\sigma_{xx}-\sigma_{yy}\right)^2 + 2L\sigma_{yz}^2 + 2M\sigma_{zx}^2 + 2N\sigma_{xy}^2 = \bar{\sigma}^2$$

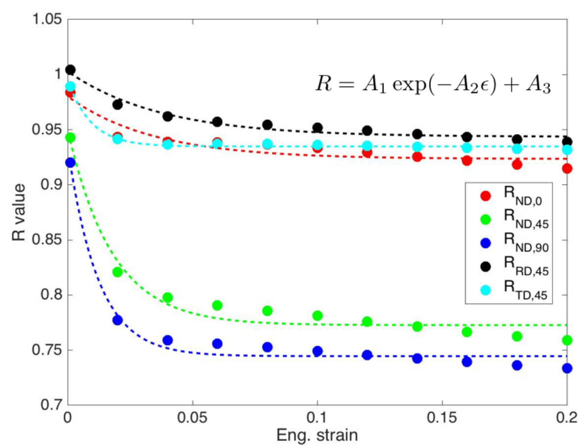
$$F = \frac{r_{ND,0}}{r_{ND,90}\left(1+r_{ND,0}\right)} \qquad L = \frac{1}{2}\left(1+2r_{RD,45}\right)$$

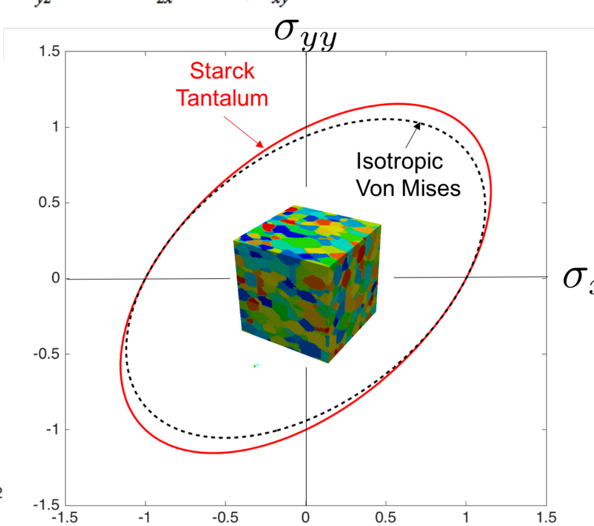
$$G = \frac{1}{1+r_{ND,0}} \qquad M = \frac{\left(r_{ND,0}+r_{ND,0}r_{ND,90}\right)\left(2r_{TD,45}+1\right)}{2r_{ND,90}\left(1+r_{ND,0}\right)}$$

$$H = \frac{r_{ND,0}}{1+r_{ND,0}} \qquad N = \frac{\left(r_{ND,0}+r_{ND,90}\right)\left(2r_{ND,45}+1\right)}{2r_{ND,90}\left(1+r_{ND,0}\right)}$$

F	*G*	*H*	*L*	*M*	*N*
0.62	0.52	0.48	1.43	1.59	1.42

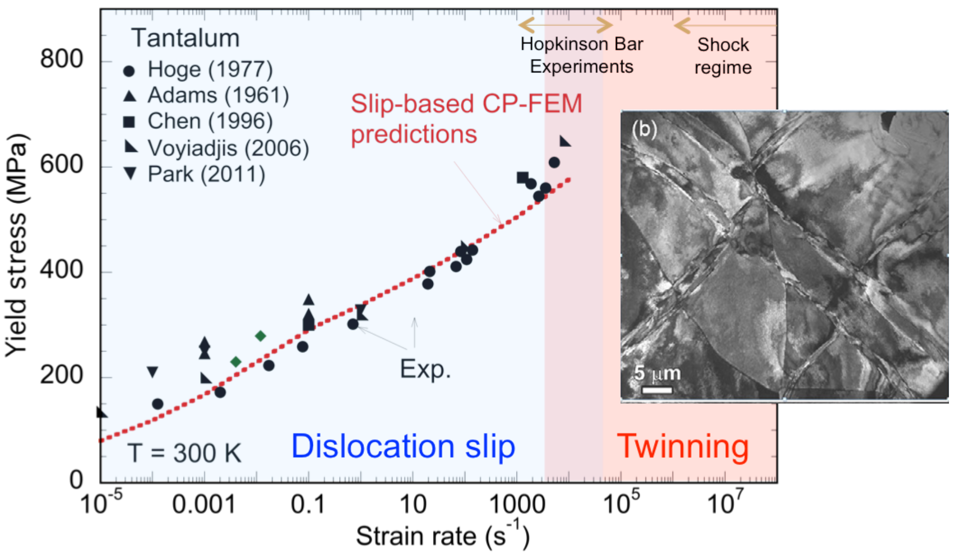
Anisotropy calculation

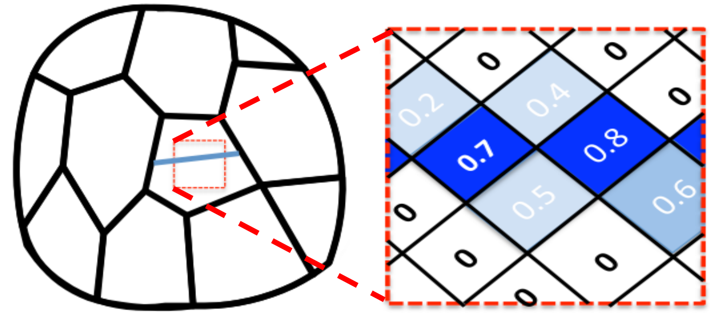




Anisotropic yield model is constructed using measured texture (EBSD) and crystal plasticity models. Developed anisotropic model can be used in continuum scale models to accurate model anisotropic behaviors in engineering scale components.

Deformation twinning in Tantalum: Volume fraction model



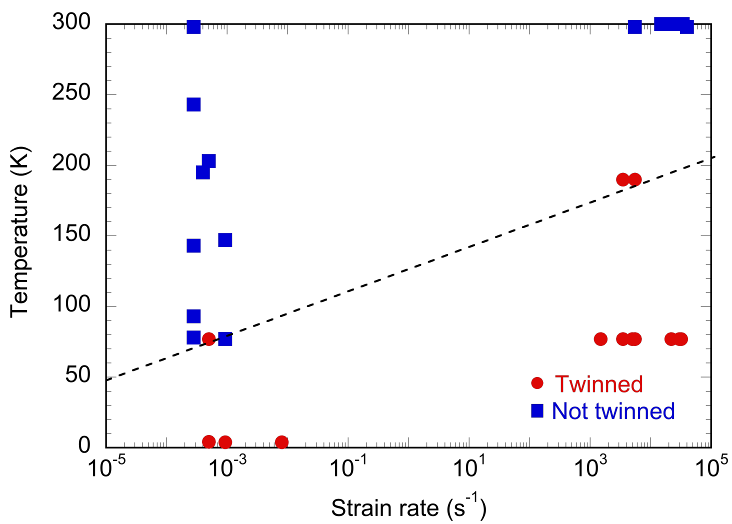


Polycrystalline body

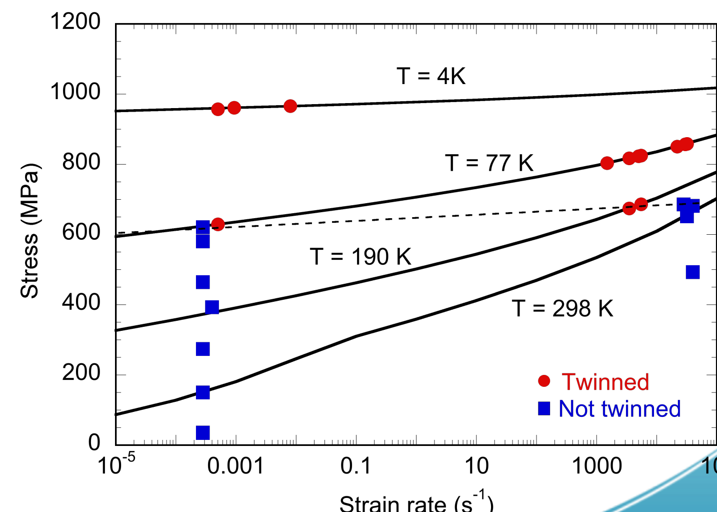
Volume fraction model

$$\mathbf{L}^p = \left(1 - \sum^{N^{tw}} f^\beta\right) \sum^{N^s} \dot{\gamma}^\alpha \mathbf{S}^\alpha_{o,s} + \sum^{N^{tw}} \dot{f} \gamma^t \mathbf{S}^\alpha_{o,tw} + \sum^{N^{tw}} f^\beta \sum^{N^{t,s}} \dot{\gamma}^\alpha \mathbf{S}^\alpha_{t,s}$$

Slip in untwinned region | twinning | Slip in twinned region



Experimental observation of twinning



Stress required to initiate twinning

Additional slides

Using scaling to discern strain-rate dependence

Scaling conditions for loading:

$$v(t) = v'(t') \qquad \& \qquad t' = \frac{1}{M}t$$

$$x'\left(\frac{1}{M}t\right) = \frac{1}{M}x(t)$$

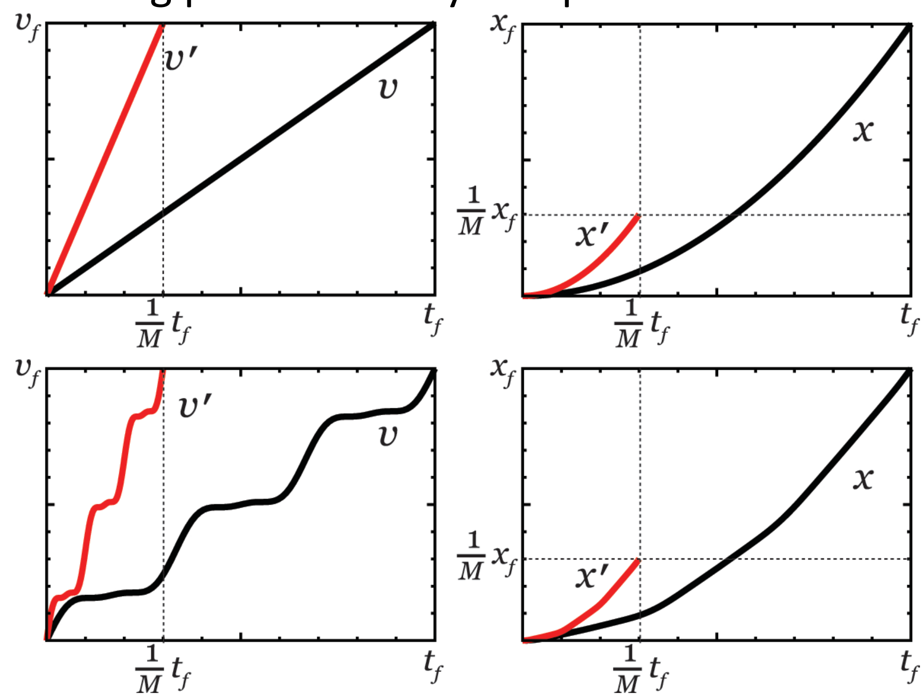
$$v'\left(\frac{1}{M}t\right) = v(t)$$

Dynamic similarity:

$$\frac{F_{\mathrm{model}}}{F_{\mathrm{actual}}} = \frac{M_{\mathrm{m}}\frac{L_{\mathrm{m}}}{T_{\mathrm{m}}^2}}{M_{\mathrm{a}}\frac{L_{\mathrm{a}}}{T_{\mathrm{a}}^2}} = \frac{\rho_{\mathrm{m}}A\frac{L_{\mathrm{m}}^2}{T_{\mathrm{m}}^2}}{\rho_{\mathrm{a}}A\frac{L_{\mathrm{a}}^2}{T_{\mathrm{a}}^2}}$$

$$= \lambda_\rho\left(\frac{\lambda_L}{\lambda_T}\right)^2 = 1$$

Driving piston velocity and position:



Invariant to scaling:

Velocity Stress
Strain Temperature*
Forces Density

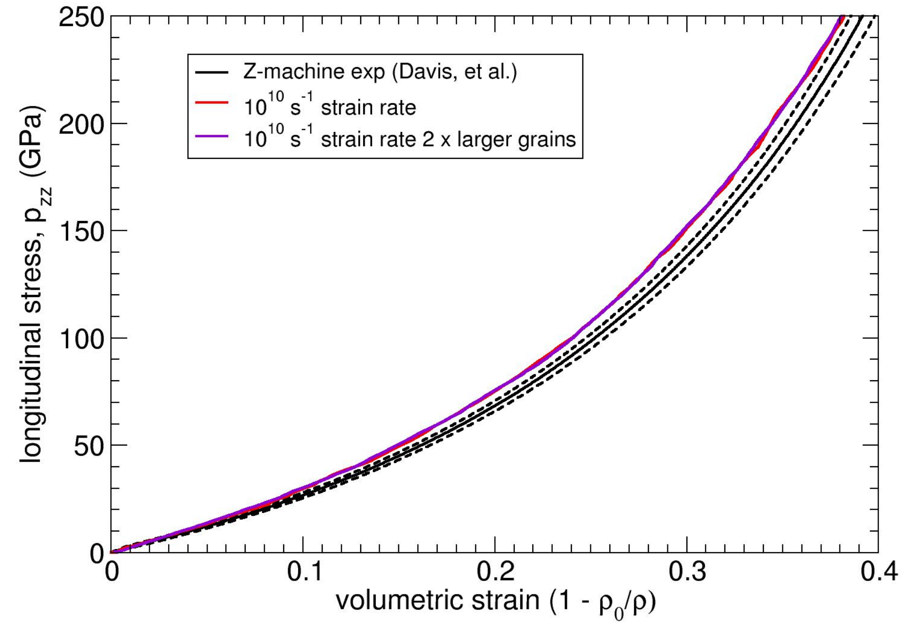
Not invariant:

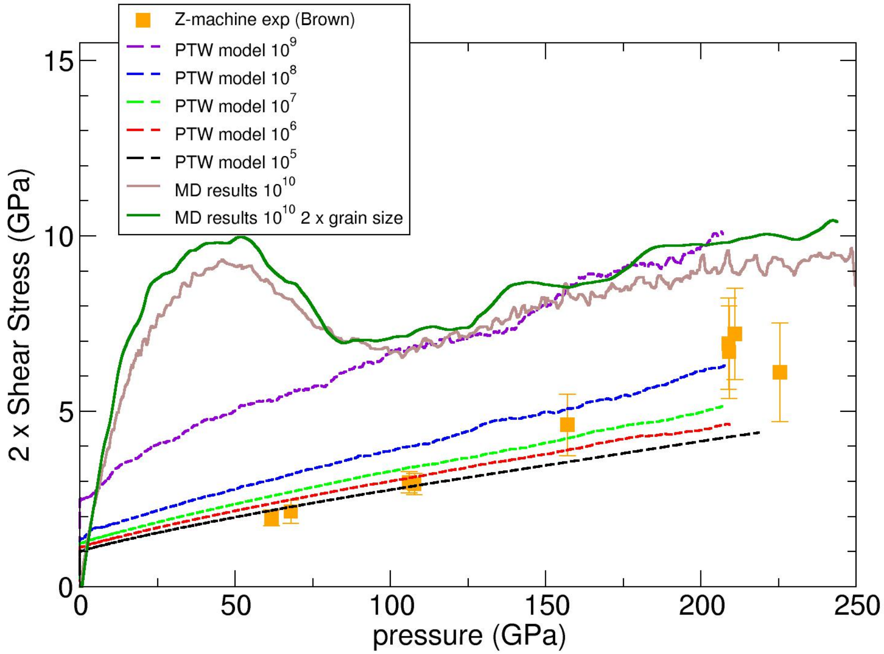
Strain rates
Accelerations
Times and distances
any extensive variable…

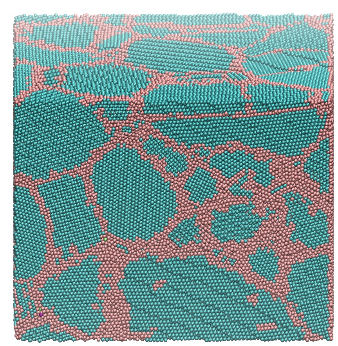
Increased grain size

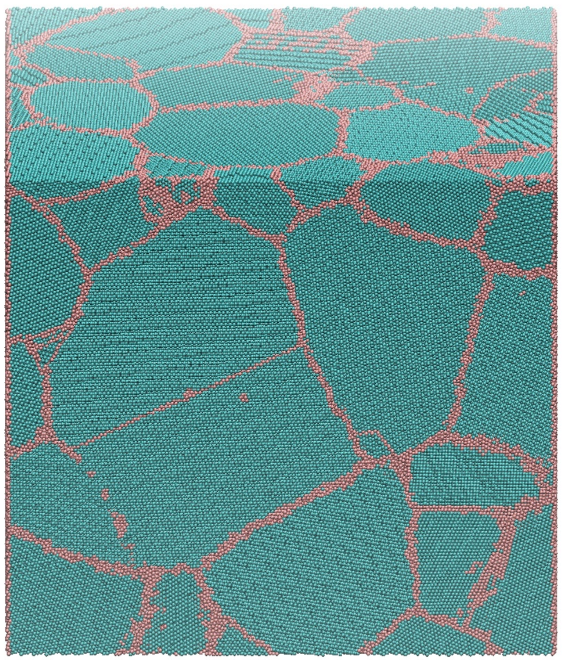
Increasing grain size by a factor of two, to 8-20 nm confirms an inverse Hall-Petch response

At high strain rates the stress-strain relations are not impacted by grain size, while strength is marginally increased.







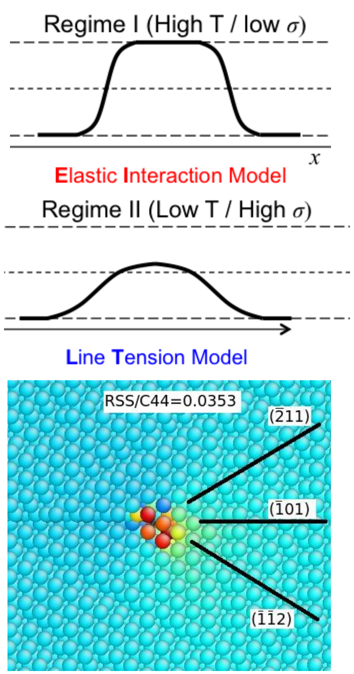


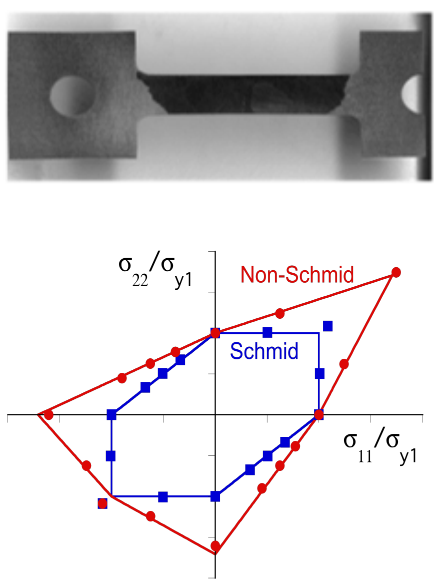
Matthew Lane - jlane@sandia.gov

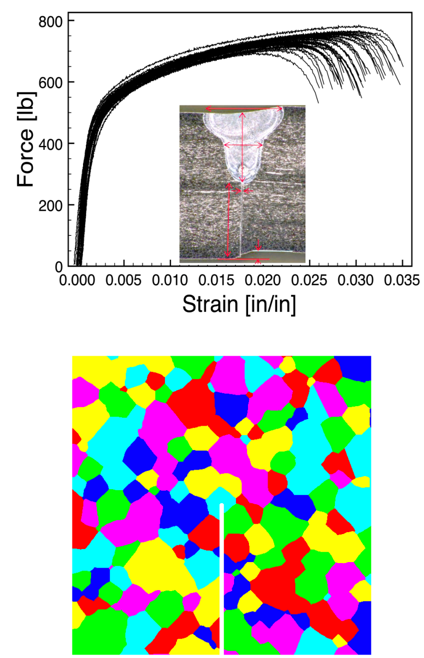
Overview: Multi-scale Approach

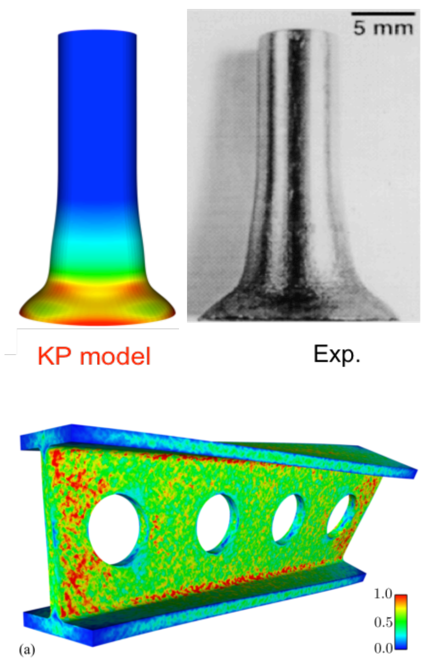
Multi-scale simulations & experiments to predict material's reliability

Atomic scale phenomena	Single crystal behavior	Microstructural effects	Material Performance
10^{-9} m	10^{-6} m	10^{-3} m	10^{0} m









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